

Benzo[a]carbazole

Other names:	Benzo[a]carbazole 1,2-Benzcarbazole 1,2-Benzocarbazole 11-Azachrysofluorene
Inchi:	InChI=1S/C16H11N/c1-2-6-12-11(5-1)9-10-14-13-7-3-4-8-15(13)17-16(12)14/h1-10,17H
InchiKey:	MYKQKWIPLZEVOW-UHFFFAOYSA-N
Formula:	C16H11N
SMILES:	<chem>c1ccc2c(c1)ccc1c3ccccc3[nH]c21</chem>
Mol. weight [g/mol]:	217.27

Physical Properties

Property code	Value	Unit	Source
hf	276.11	kJ/mol	Cheméo Relay (1.0)
hvap	109.66	kJ/mol	Cheméo Relay (1.0)
ie	7.10 ± 0.10	eV	NIST Webbook
log10ws	-5.94		Cheméo Relay (1.0)
logp	3.992		Crippen Method
mcvol	168.440	ml/mol	McGowan Method
pc	3260.93	kPa	Cheméo Relay (1.0, beta)
rinpol	400.00		NIST Webbook
rinpol	401.81		NIST Webbook
rinpol	402.22		NIST Webbook
rinpol	403.50		NIST Webbook
tb	705.47	K	Cheméo Relay (1.0)
tc	1027.64	K	Cheméo Relay (1.0)
tf	518.49	K	Cheméo Relay (1.0)
vc	0.649	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C239010&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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